Suppression of Premixed C_3H_8-Air Flames by Halogenated and Phosphorus-Containing Compounds

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ABSTRACT

Calculations were performed using the HCT (Hydrodynamics, Chemistry and Transport) code to investigate the means by which different suppressants act on a premixed, propane/air flame. Two classes of suppressants are investigated: halogenated, HBr, CF_3Br, and phosphorus-containing compounds, dimethyl methylphosphonate (DMMP) and sarin ($POFCH_3OC_3H_7$). Although investigations of these compounds has been performed by various authors, no known previous work has been performed to directly compare the suppression mechanism between the halogenated compounds (HBr and CF_3Br) and phosphorus-containing compounds, or PCCs (DMMP and sarin) in a premixed flame. Of particular interest is a comparison of the location in the flame that the suppressant act. It has been shown that for phosphorus-containing compounds, radical recombination reactions reduce radical concentrations near the post-flame region, as opposed to the halons which primarily exhibit recombination in the pre-flame zone. This behavior leads to the greater effectiveness of the organophosphorus suppressant compared to the halogenated suppressants.

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INTRODUCTION

Motivation

- Halons and phosphorus-containing compounds (PCCs) are chemically active flame inhibitors in that they catalytically recombine key flame radicals (H, O, OH).
- PCCs are more effective than halons, but why?
  - More effective radical scavengers?
  - Does location where radical recombination occurs matter in a premixed flame?
- How do PCCs compare to a "perfect" inhibitor (as described by Rumminger, *et al*, 2003)?

Modeling Approach

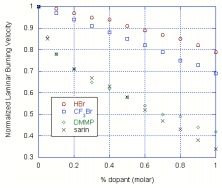
- HCT code was used to model freely propagating, premixed, stoichiometric, C_3H_8/Air flame at atmospheric pressure.
- Numerically tested four compounds
  - Halons: HBr, CF_3Br
  - PCCs: Dimethyl methylphosphonate (DMMP) $[POCH_3(OCH_3)_2]$, Sarin (GB) $[POFCH_3(OC_2H_7)]$
- Hydrocarbon mechanism supplemented by dopant mechanism.
  - HBr and CF_3Br from Westbrook (1983)
  - DMMP and sarin from Glaude, *et al.* (2002)

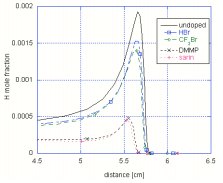
Inhibition Mechanism

- HBr reduces H concentration via:
  - $H + HBr \rightarrow H_2 + Br$
  - $H + Br_2 \rightarrow HBr + Br$
  - $Br + Br \rightarrow Br_2$
- DMMP reduces H concentration via:
  - $H + PO_2 \rightarrow HOPO$
  - $H + HOPO \rightarrow H_2 + PO_2$
- Reduction in H translates to a reduced reaction rate. $H + O_2 \rightarrow OH + O$

➢ Overall reduction in flame propagation

RESULTS

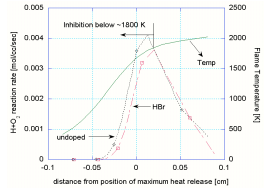


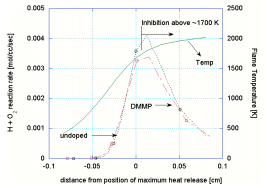


Inhibition Effectiveness

Sarin > DMMP > CF_3Br > HBr

- PCCs several times more effective than halons.
  - Greater reduction in laminar burning velocity as a function of loading.
  - Greater reduction in concentration of H radicals across flame for a given loading.
- Further support that the form of parent PCC is relatively unimportant in effectiveness.
- Sarin and CF_3Br have extra activity of fluorine.
- Non-linear behavior of PCCs not well understood.





Recombination Temperature

- Rumminger, *et al*. (2003)* found that:
  - A "perfect" inhibitor acts at high temperatures (1700-2150 K).
  - CF_3Br is not as effective since most recombination occurs at low temperatures (<1800 K).
- Our results show that:
  - HBr and CF_3Br cause recombination of H at fairly low temperatures <1800 K.
  - DMMP and sarin cause recombination of flame radicals at high temperatures >1700 K.

SUMMARY & CONCLUSIONS

- Location in premixed flame at which suppressants act is not the same for halons and PCCs.
  - Halons recombine radicals in pre-flame region.
  - PCCs recombine radicals in high temp region.
- This behavior indicates that PCCs tend toward being "perfect" inhibitors, as described by Rumminger,*et al*. (2003)*.
- Further support that PCCs are effective suppressants and form of parent PCC is relatively unimportant.
- Further work being performed by varying equivalence ratio.

*Ref: Rumminger, M. D., Babushok, V. and Linteris, G. T., *Proc. Combust. Inst.* 29: 329-336 Part 1 (2003).